Revisiting "swings" in the crossover features of Ising thin films near $T_c(D)$

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"Swing" effects at the onset of crossover towards two dimensional behavior in thin Ising films are investigated close to $T_c(D)$ by means of Monte Carlo calculations. We find that the effect is extremely large for the specific heat effective critical exponent, in comparison with the "swing" already noted by Capehart and Fisher for the susceptibility. These effects change considerably the system's evolution with thickness (D) from two-dimensional to three-dimensional behavior, forcing the effective exponents to pass near characteristic Tri Critical Point (TCP) values.

Basic features of phase transitions in systems with thin film geometry have been connected with the problem of the crossover from classical to quantum transitions. The change from classical to quantum character of the transition can be mapped to the evolution with thickness of the phase transition in films (se f.i. [1,2]).That is the reason why a detailed study of phase transitions in films may be particularly useful for the study of quantum phase transitions apart from the intrinsic usefulness of studying changes in systems with a few layers of thickness. The effective critical exponents and the evolution near the critical point has been extensively studied by means of series expansions [3], the renormalization group [4], and Monte Carlo calculations in Ising systems [5], as well as in the X-Y model [6]. For systems with thin film geometry, the correlation length is much smaller than the film thickness (D), sufficiently below and above the critical point (i.e. relatively far from $T_c(D)$). Once the correlation length grows sufficiently (i.e. close to $T_c(D)$) the system notices that its critical behavior cannot be that of a three-dimensional system and the crossover to the two-dimensional behavior begins. From the point of view of the **effective critical exponents** this means that the system is initially evolving towards **three-dimensional** behavior until a crossover to **two-dimensional** behavior takes place. The film thickness can be characterized by the value of the effective critical exponents just at the onset of this crossover.

The pioneering work of Capehart and Fisher [3] noted that for the case of the effective critical exponent corresponding to the susceptibility (γ_{eff}) an **"under-swing"** behavior was apparent just before the crossover. This characteristic behavior means that for a certain thickness D^* the effective critical exponent reaches a minimum with a value $\gamma_m(D^*) < \gamma^{3D} < \gamma^{2D}$. This kind of behavior was attributed to surface effects, due to the lower value of the thickness ($D << L$). In principle one might expect to find an enhancement of the pehenomenon using **free** boundary conditions in comparison with **periodic** boundary conditions, as indeed it was seen the case.

Since that time there has not been much work on the problem considered because research has been devoted strictly to the very close vicinity of the critical point. Monte Carlo simulations [5] have shown the existence of this "under-swing", but no attempt has been made to characterize this phenomenon. In principle this "under-swing"is a small effect, since $\gamma_m(D^*)$ is close to γ^{3D}, but several very interesting questions can be asked concerning this phenomenon: a) We know that there should be a value of the thickness D for which this effect should be maximum, D^*, because eventually γ_{eff} must increase again as ($D \to L$) towards γ^{3D}: What is the value D^* of this characteristic thickness? b) Is it possible to get more pronounced "swing" effects in other critical exponents?, c) What are the values of these effective critical exponents for D^* corresponding to the maximum "swing"? d) Is there a substantial difference between the exponent values obtained using **periodic** and **free** boundary conditions?

In the present work we will address these questions studying the thickness dependence of the **effective critical exponents** (β_{eff}, γ_{eff}, δ_{eff}, α_{eff}) of Ising film ($L \times L \times D$), describing the evolution from the pure two-dimensional Ising system ($D = 1$) towards the three-dimensional system ($D = L$) system. In order to obtain the actual behavior of the effective critical exponents we will make use of the fact that the scaling relations hold all the way before and all through the crossover region

FIG. 1. Evolution of the effective critical exponents with temperature for different thickness D=3 (squares), D=5 (circles) and D=9 (triangles) with periodic (full) and free (open) boundary conditions. Two dimensional and three dimensional critical exponents are marked (full lines) together with the Tri Critical Point values (dashed line). The arrows indicate the "under-swing" (b) and "over-swing" (d) behavior.

The "under-swing" effect noted by Capehart and Fisher [3] is explicit for the case of the susceptibility. In order to check this effect, we present in Fig 1b results for γ_{eff} vs. $log[T_c(D) - T]$ for $D = 3, 5, 9$. Note how the "under-swing" is clearly detectable for values of D close to $D = 9$. This "under-swing" is visible not just for the free boundary conditions, but also for the periodic boundary conditions as was pointed out in Ref. [3]. This is the first time in our knowledge that the "under-swing" effect is explicitly shown to exist under periodic boundary conditions, where surface effects are reduced.

In order to get a more complete picture of the depen-

FIG. 2. Effective critical exponents at the onset of the crossover vs. thickness for periodic (full) and free (open) boundary conditions. Two dimensional and three dimensional critical exponents are marked (full line) together with the Tri Critical Point value (dashed line). The arrows indicate the "under-swing" in γ_{eff} (a) and "over-swing" in α_{eff} (b).

Now we focus attention on the exponent values obtained for $D = 9 \approx D^*$. The results for periodic and free boundary conditions are presented in Table I. They are compared with the **two-dimensional** values, the **three-dimensional** values and with the **Tri Critical Point** (TCP) values. As it is known, a Tri Critical Point is at the limit separating **continuous** (2^{nd} order) from **discontinuous** (1^{st} order) transitions [13]. Note that the exponent values corresponding to the Tri Critical Point are close to those for $D = 9 \approx D^*$, with errors ranging from three to twelve percent. Clearly, the evolution of the effective critical exponents $[\beta_m(D), \alpha_m(D), 1/\delta_m(D)$ and $\gamma_m(D)]$ from the two-dimensional values ($D = 1$) to the three-dimensional values ($D = L$) is not monotonous but appears in all cases to come close to the respective Tri Critical Point value for $D \approx D^*$. This effect is made more explicit in plots of $\alpha_m(D)$ vs. $\gamma_m(D)$ and $1/\delta_m(D)$ vs. $\beta_m(D)$ (see Fig.3a and 3b).

FIG. 3. Evolution of the effective critical exponents at the onset of the crossover as the thickness of the system increases for periodic (full) and free (open) boundary conditions. The straight dashed line indicates a linear evolution, and the full line is a guide for the eye indicating the observed evolution. Note that the effective exponents tend towards the Tri Critical Point values (marked with an cross). Dotted lines indicate the expected behavior towards the three-dimensional value.

Fig.3a shows that, in the case of $\alpha_m(D)$ vs. $\gamma_m(D)$,the evolution of the plot from $D << D^*$ $[\gamma_m(D) \sim \gamma^{2D}, \alpha_m(D) \sim \alpha^{2D}]$ onwards shows an spectacular turn towards the **Tri Critical Point** pair of values $(\gamma^{TCP}, \alpha^{TCP})$. Then for $D > D^*$ the evolution towards the pure three-dimensional values begins. Note that the data points get away from the box defined by $(\gamma^{2D}, \alpha^{2D}) \iff (\gamma^{3D}, \alpha^{3D})$, making explicit the existence of "swing effects". An interesting feature of our results is that the general behavior appears to follow the same well defined line independently of the boundary conditions used.

For the case of $1/\delta_m(D)$ vs. $\beta_m(D)$ the values corresponding to a Tri Critical Point are also closely approached. The non-existence of swing effects in this case is also explicit since the pair of values $(\beta_m(D), 1/\delta_m(D))$ do not leave the box.

In conclusion we have presented Monte Carlo data for the evolution of **effective critical exponents** (note that these are "transient" exponents, not assyntotic, critical exponents) in thin Ising films. In summary we have shown that: a) "Swing effects" are specially enhanced for the specific heat effective exponent, $\alpha_m(D)$, b) They appear very clearly for both free and periodic boundary conditions and c) "Swing effects" force the effective exponents to pass near exponent values corresponding to a Tri Critical Point (for $D^* \simeq 10$) well before the evolution towards the three-dimensional values begins.

Our work shows that "swing" effects must become patent especially in the case of the specific heat for any boundary conditions. It would be very interesting to check this point experimentally. This result rises also the basic question of **why** Tri Critical Point exponents $(\beta = 1/4, 1/\delta = 1/5, \gamma = 1, \alpha = 1/2)$ describe so well the behavior of thin films at the onset of the crossover, for characteristic thicknesses of $D^* \simeq 10$.

TABLE I. Effective critical exponents for Ising films at onset of crossover and $D \simeq D^*$

	β	γ	$1/\delta$	α
Two Dimensional	0.125	1.75	0.066	0.000
D=9 (periodic)	0.218	1.13	0.152	0.469
D=9 (free)	0.243	1.06	0.174	0.525
Tri Critical Point	0.250	1.00	0.200	0.500
Three Dimensional	0.330	1.24	0.208	0.110

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